

What is claimed is:

1. The crystalline complex comprising *T. foetus*
IMPDH in complex with inosine monophosphate (IMP), having
5 atomic coordinates set forth in Table 2.

2. The crystalline complex comprising *T. foetus*
IMPDH in complex with inosine monophosphate (IMP) and
mycophenolic acid, having atomic coordinates set forth in
10 Table 3.

3. The crystalline complex comprising *T. foetus*
IMPDH in complex with xanthosine monophosphate (XMP) and
mycophenolic acid, having atomic coordinates set forth in
15 Table 4, the IMPDH having a complete active site.

4. The crystalline complex comprising *T. foetus*
IMPDH in complex with xanthosine monophosphate (XMP) and
nicotinic adenine dinucleotide (NAD), having atomic
20 coordinates set forth in Table 5.

5. The crystalline complex comprising *T. foetus*
IMPDH in complex with ribovirin (1- β -D-ribofuranosyl-
1,2,4-triazole-3-carboxamide, having atomic coordinates
25 set forth in Table 7.

6. The crystalline complex comprising *T. foetus*
IMPDH in complex with ribovirin and mycophenolic acid,
having atomic coordinates set forth in Table 6.

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7. Atomic coordinates for the bound complex of *T. foetus* IMPDH with inosine monophosphate (IMP), having atomic coordinates set forth in Table 2.

5 8. Atomic coordinates for the bound complex of *T. foetus* IMPDH with IMP and mycophenolic acid having atomic coordinates set forth in Table 3.

9. Atomic coordinates for the bound complex of *T. foetus* IMPDH with xanthosine monophosphate (XMP) and mycophenolic acid set forth in Table 4.

10. Atomic coordinates for the bound complex of *T. foetus* IMPDH with xanthosine monophosphate (XMP) and
15 nicotinic adenine dinucleotide (NAD) set forth in Table
5.

11. Atomic coordinates for the bound complex of *T. foetus* IMPDH with ribovirin (1- β -D-ribofuranosyl-1,2,4-
20 triazole-3-carboxamide set forth in Table 7.

12. Atomic coordinates for the bound complex of *T. foetus* IMPDH with ribovirin and mycophenolic acid set forth in Table 6.

13 A method of identifying an inhibitor of IMPDH, comprising:

- 5 (a) displaying a structure for IMPDH, or a portion thereof, wherein the structure has a set of atomic coordinates shown in Tables 2-7;
- (b) docking a structure of a candidate inhibitor to the structure of IMPDH, or the portion thereof; and
- 10 (c) identifying an inhibitor of IMPDH, wherein the inhibitor has a structure that docks favorably to the structure of IMPDH, or the portion thereof

14. The method of claim 13, wherein inhibitor that targets the substrate binding site to which IMP or XMP
15 bind is identified.

15. The method of claim 13, wherein an inhibitor that targets the NAD cofactor binding site to which NAD or MOA bind is identified.

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16. The method of claim 13, further comprising docking a candidate inhibitor to a second IMPDH structure.

17. A method of identifying an inhibitor of IMPDH, comprising:

(b) displaying the structure for the bound complex
5 of *T. foetus* inosine monophosphate dehydrogenase with NAD set forth in Table 5, (b) docking a structure of a candidate inhibitor to said structure, or portion thereof; and

(c) identifying a compound that binds Asp-358 and
10 Asp-261, wherein said compound has a structure that docks favorably to said structure, or portion thereof.

18. A method of identifying an inhibitor of IMPDH, comprising:

15 (a) selecting a candidate compound by performing rational drug design with a set of atomic coordinates set forth in Tables 2-7, wherein said selecting is performed in conjunction with computer modeling;

(b) contacting said compound with IMPDH, and

20 (c) determining the ability of said compound to reduce IMPDH activity,

wherein a compound that reduces IMPDH activity is an inhibitor of IMPDH.